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Effects of Electron Correlation near Spin-Density-Wave on Angle Dependence of Magnetoconductivity

Hirono Kaneyasu*, Keita Kishigi[1] and Yasumasa Hasegawa

Department of Material Science, University of Hyogo, Kamigori, Akou, Hyogo 678-1297, Japan
[1]*Department of Education, Kumamoto University, Kumamoto 860-8555, Japan*

The effect of electron correlation on the angle dependence of magnetoconductivity is studied in quasi-one-dimensional organic conductors. We investigated the effect on the basis of the momentum dependence of both quasi-particle's lifetime and velocity near the spin-density-wave (SDW). We found that the momentum dependence of quasi-particle's lifetime mainly governs the angle dependence of one-dimensional axis magnetoconductivity. On the other hand, the change in velocity originating from the electron correlation gives the dominant effects on the angle dependence of the interchain axis magnetoconductivity. The effect of electron correlation is clarified from the association of the momentum dependences of lifetime and velocity with the momentum dependences of commensurate orbitals on a Fermi surface in magnetic fields.

KEYWORDS: magnetconductivity, electron correlation, angle dependence, one-dimensional organic conductor, spin-density-wave

Quasi one-dimensional (Q1D) organic conductors often show spin-density-wave (SDW) and field-induced SDW, which are caused by strong electron correlation (EC).[1,2] In these systems, the angle-dependent magnetoresistance oscillation (AMRO) has been discovered as a profitable study for the fermiology of low-dimensional conductors (TMTSF)$_2$X.[3–5] Experimentally, minimums at magic angles are observed in both 1D axis and interchain magnetoresistances in the magnetic fields in a $y-z$ plane.[3–5] Here, the magic angles θ of a magnetic field are given from the relation of $\theta = \tan^{-1}(\frac{p}{q})$, where p and q are integers.[3–5] The electron has commensurate routes on a Fermi surface (FS) at magic angles, whereas it has incommensurate routes at other angles. The strong angle dependence of interchain magnetoresistance was obtained in terms of the topology of the linearized dispersion in the k_x-direction on FS.[6,7]

On the other hand, the angle dependence of the 1D axis magnetoresistance is not obtained from the linearized FS because a 1D axis velocity has no momentum dependence. Although the angle dependence of 1D axis magnetoresistance is obtained from the unlinearized dispersion on the FS, it is much weaker than that observed experimentally.[8] It is found that the angle dependence of 1D axis magnetoconductivity (σ_{xx}) appears when a spot of slow or fast velocity exists in the momentum space of the 1D axis velocity.[9] The result in this simple model indicates the possibility that the change in velocity near SDW causes the strong angle dependence in σ_{xx}.

As for another mechanism, the effect of Umklapp scattering[10] near SDW was considered on the basis of the momentum dependence of scattering rate[11–14] in the linearized dispersion on FS. Lebed and Bak[11] have first pointed out that magnetoresistance in Q1D organic systems depends on the angles of the magnetic field by studying the effect of EC with impurities. They obtained, however, the peaks of magnetoresistivity at magic angles, instead of the dips (i.e., peaks of magnetoconductivity) observed in experiments. Zhelenznyak and Yakovenko[13] have studied the field angle dependence of both 1D axis and interchain magnetoresistance in Q1D organic systems in a strong magnetic field on the basis of the semiclassical Boltzmann theory by taking account of the momentum-dependent scattering rate due to the topology of the Q1D FS. Yanase and Yamada[17] have studied the $c-$axis resistivity in quasi two-dimensional cuprate systems on the basis of the semiclassical Boltzmann theory, where both energy and the lifetime of quasi-particle are obtained using the second order perturbation theory in the on-site repulsion. Their study is performed only in zero magnetic field.

Here, we study σ_{xx} and interchain magnetoconductivity (σ_{zz}) in the Q1D organic systems in the strong magnetic field tilted in the $y-z$ plane on the basis of the semiclassical Boltzmann theory by considering the effect of EC on both lifetime and energy (and its derivative, the velocity of quasi-particle) in a random phase approximation (RPA). The effect of EC is treated in the full momentum dependence with the unlinearized dispersion. Because spin susceptibility is expected to be strongly affected by EC in the Q1D organic systems, which are close to SDW instability, the effect of EC is analyzed using the more appropriate RPA than the second order perturbation theory.

As for formulation, the dispersion of a tight-binding model is given by $E_{\mathbf{0}}(\mathbf{k}) = -2t_a \cos k_x - 2t_b \cos k_y - 2t_c \cos k_z$, where the nearest-neighbor hopping parameters are $t_a = 1.0$ and $t_b = t_c = 0.1$ for the simplified Q1D FS of organic conductors. We use t_a as the unit of energy. The realistic parameters for (TMTSF)$_2$X are $t_b = 0.1$ and $t_c = 0.03$. However, we use the symmetric parameter $t_b = t_c = 0.1$ for the saving of three-dimensional mesh in momentum space. Electrons are set to be quarter-filled. The self-energy $\Sigma(\mathbf{k}, \omega_n)$ is obtained on the basis of RPA with respect to the on-site interaction U in the Hubbard

*E-mail hirono@sci.u-hyogo.ac.jp

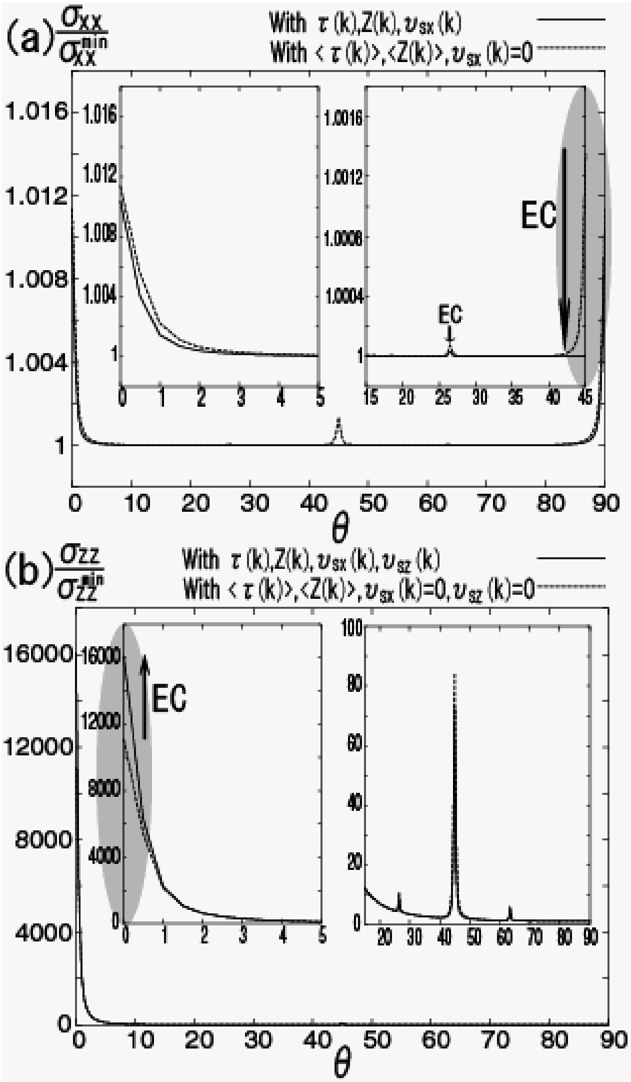

Fig. 1. (a) Angle dependence of σ_{xx}. (b) Angle dependence of σ_{zz}. The solid lines mean the magnetoconductivities with using the momentum dependent $\tau(\mathbf{k})$, $Z(\mathbf{k})$ and $\upsilon_{sx}(\mathbf{k})$ (and $\upsilon_{sz}(\mathbf{k}) in (b)$). The dash lines indicate the magnetoconductivies in the case that we neglect the momentum dependence of $\tau(\mathbf{k})$, $Z(\mathbf{k})$ and $\upsilon_{sx}(\mathbf{k})$ (and $\upsilon_{sz}(\mathbf{k})$ in (b)) by using $\langle\tau(\mathbf{k})\rangle$, $\langle Z(\mathbf{k})\rangle$, and $\upsilon_{sx}(\mathbf{k}) = 0$ (and $\upsilon_{sz}(\mathbf{k}) = 0$ in (b)).

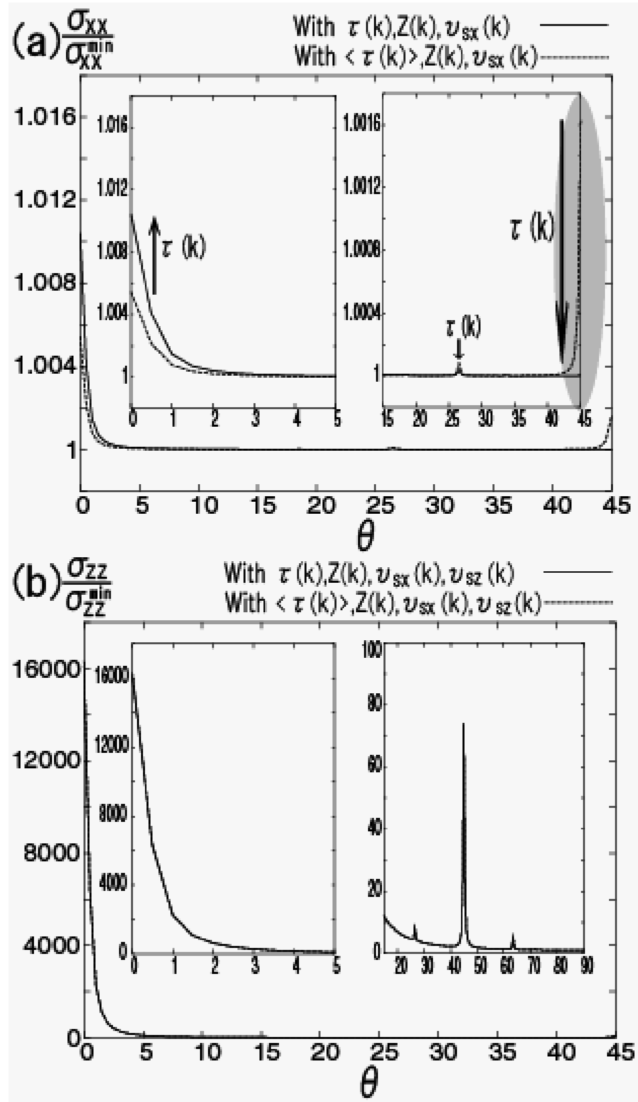

Fig. 2. (a) Angle dependence of σ_{xx}. (b) Angle dependence of σ_{zz}. The solid lines mean the magnetoconductivities with using the momentum dependent $\tau(\mathbf{k})$, $Z(\mathbf{k})$, $\upsilon_{sx}(\mathbf{k})$ and $\upsilon_{sz}(\mathbf{k})$. The dash lines indicate the magnetoconductivities in the case that the momentum dependence of $\tau(\mathbf{k})$ is neglected by using $\langle\tau(\mathbf{k})\rangle$. In σ_{zz} in (b), two lines are overlapped and indistinguishable on the scale.

model. $\Sigma(\mathbf{k},\omega_{\rm n})$ is given by

$$\Sigma(\mathbf{k},\omega_{\rm n}) = \frac{T}{N}\sum_{\mathbf{k}',m} U^2[\frac{3}{2}\chi_s(\mathbf{k}',\omega_{\rm m}) + \frac{1}{2}\chi_c(\mathbf{k}',\omega_{\rm m}) - \chi_0(\mathbf{k}',\omega_{\rm m})]G_0(\mathbf{k}-\mathbf{k}',\omega_{\rm n-m}). \tag{1}$$

Here, spin and charge susceptibilities are respectively $\chi_s(\mathbf{k}',\omega_{\rm m}) = \frac{\chi_0(\mathbf{k}',\omega_{\rm m})}{1-U\chi_0(\mathbf{k}',\omega_{\rm m})}$ and $\chi_c(\mathbf{k}',\omega_{\rm m}) = \frac{\chi_0(\mathbf{k}',\omega_{\rm m})}{1+U\chi_0(\mathbf{k}',\omega_{\rm m})}$ with $\chi_0(\mathbf{k}',\omega_{\rm m}) = -\frac{T}{N}\sum_{\mathbf{k},n} G_0(\mathbf{k}+\mathbf{k}',\omega_{\rm n+m})G_0(\mathbf{k},\omega_{\rm n})$, where N is the number of sites and $\omega_n = \pi T(2n+1)$ is the fermion Matsubara frequency with temperature T. The quasi-particle's velocity

$$\upsilon_i(\mathbf{k}) = \upsilon_{0i}(\mathbf{k}) + \upsilon_{si}(\mathbf{k}) = \frac{\partial E_0(\mathbf{k})}{\partial k_i} + \frac{\partial Re\Sigma^R(\mathbf{k},E^*)}{\partial k_i}, \tag{2}$$

the quasi-particle's lifetime

$$\tau(\mathbf{k}) = -\frac{1}{Im\Sigma^R(\mathbf{k},E^*)}, \tag{3}$$

and the renormalization factor

$$Z(\mathbf{k}) = \frac{1}{1 - \frac{\partial Re\Sigma^R(\mathbf{k},E)}{\partial E}|_{E=E^*}} \tag{4}$$

are given on FS. Here, i indicates x, y and z. $\Sigma^R(\mathbf{k},E^*)$ and $E^*(\mathbf{k})$ indicate a retarded self-energy and a quasi-particle's energy on FS, respectively. The angle dependence of magnetoconductivity is calculated from the Boltzmann transport theory[18] and the equation of motion in magnetic field B, $\sigma_{ij}(\theta) = \frac{e^2}{4\pi^3}\int -\frac{\partial f(E(\mathbf{k}(0)))}{\partial E}|_{E=E^*}\tilde{\upsilon}_i(\mathbf{k}(0)) \int_{-\infty}^{0}\tilde{\upsilon}_j(\mathbf{k}(t))$ $\exp[-\int_t^0 \frac{dt'}{\tilde{\tau}(\mathbf{k}(t'))}]dtd\mathbf{k}(0)$. Here, $\tilde{\upsilon}_i(\mathbf{k}(t))$ and $\tilde{\tau}(\mathbf{k}(t))$ are

$\tilde{\upsilon}_i(\mathbf{k}(t)) = Z(\mathbf{k}(t))\upsilon_i(\mathbf{k}(t))$ and $\tilde{\tau}(\mathbf{k}(t)) = \frac{\tau(\mathbf{k}(t))}{Z(\mathbf{k}(t))}$, respectively. $f(E(\mathbf{k}))$ is the Fermi distribution function. $-\frac{\partial f(E(\mathbf{k}(0)))}{\partial E}|_{E=E^*}$ is the density of states on FS. We use the relation given by $-\frac{\partial f(E(\mathbf{k}(0)))}{\partial E}|_{E=E^*} = \frac{1}{\tilde{\upsilon}_x(\mathbf{k}(0))}$ in the Q1D system. σ_{xx} $(i=j=x)$ and σ_{zz} $(i=j=z)$ are

$$\sigma_{xx}(\theta) = \frac{e^2}{4\pi^3}\int\int_{-\infty}^{0}\tilde{\upsilon}_x(\mathbf{k}(t))\exp[-\int_t^0\frac{dt'}{\tilde{\tau}(\mathbf{k}(t'))}]dtd\mathbf{k}(0) \tag{5}$$

and

$$\sigma_{zz}(\theta) = \frac{e^2}{4\pi^3}\int\frac{1}{\tilde{\upsilon}_x(\mathbf{k}(0))}\tilde{\upsilon}_z(\mathbf{k}(0))\int_{-\infty}^{0}\tilde{\upsilon}_z(\mathbf{k}(t)) \times\exp[-\int_t^0\frac{dt'}{\tilde{\tau}(\mathbf{k}(t'))}]dtd\mathbf{k}(0). \tag{6}$$

The equation of motion is $\hbar\frac{d\mathbf{k}(t)}{dt} = -e\tilde{\mathbf{v}}(\mathbf{k}(t))\times\mathbf{B}$, where magnetic field $\mathbf{B}$ is in the $y-z$ plane and $\mathbf{B} = (0, B\sin\theta, B\cos\theta)$. In the numerical calculation, we divide the first Brillouin zone into 64^3 momentum meshes and take the cut-off $N_f = 128$ for Matsubara frequency ω_n. The bandwidth $2W$ $(W\sim 2.2)$ is a necessary range of ω_n for reliable calculations, that is $W < \pi T N_f$. To satisfy the condition, the conductivity should be calculated in the region with $T > 0.0055t_a$. We choose the parameters as $T = 0.008$, $U = 1.98$ and $B\langle\tau(\mathbf{k})\rangle = 150$. Here, $\langle ...\rangle$ means the average on FS. The SDW state is stabilized in the region of $U > 3.1$ where $\chi_s(k)$ diverges.

In our result for the noninteracting system ($U = 0$), the peaks of σ_{zz} appear at magic angles $\theta = 0°$, $26.6°(=\tan^{-1}(\frac{1}{2}))$ and $45°(=\tan^{-1}(1))$. The angle dependence of σ_{zz} in the noninteracting system corresponds to the angle dependence due to the topology of the unlinearized dispersion on FS.[7] At $U = 0$, we obtain that the small peaks of σ_{xx} also appear at the same magic angles originating from the topology of FS. The angle dependences of σ_{xx} and σ_{zz} are equal to the angle dependence in the non-interacting system when we neglect the momentum dependence of $\tau(\mathbf{k})$, $Z(\mathbf{k})$ and $\upsilon_{sx}(\mathbf{k})$ by using $\langle\tau(\mathbf{k})\rangle$, $\langle Z(\mathbf{k})\rangle$, $\upsilon_{sx}(\mathbf{k}) = 0$ and $\upsilon_{sz}(\mathbf{k}) = 0$, as shown in Figs.1(a) and 1(b).

As show in Fig.1(a), σ_{xx} is strongly suppressed at the magic angle $\theta = 45°$ when we calculate it using the momentum dependent $\tau(\mathbf{k})$, $Z(\mathbf{k})$ and $\upsilon_{sx}(\mathbf{k})$. The effect is small at other angles $\theta = 0°$ and $26.6°$. We calculate σ_{xx} by neglecting only the momentum dependence of $\tau(\mathbf{k})$ (using the averaged value $\langle\tau(\mathbf{k})\rangle$). In this case, the peak of σ_{xx} at $\theta = 45°$ is large as show in Fig. 2(a). Therefore, we conclude that the suppression in the peak of σ_{xx} at 45° due to EC comes through the momentum dependence of $\tau(\mathbf{k})$. The region of the small value of $\tau(\mathbf{k})$ is attributed to the verge of the SDW. The region of small lifetime originates from the nesting of FS near the SDW in as shown Fig. 4(a). The effects of the momentum dependence of $\tau(\mathbf{k})$ in σ_{zz} are very small as shown in Fig. 2(b).

Figure 1(b) shows that the peak of σ_{zz} is enhanced at $\theta = 0°$ when we take the momentum dependences of $\tau(\mathbf{k})$, $Z(\mathbf{k})$, $\upsilon_{sx}(\mathbf{k})$ and $\upsilon_{sz}(\mathbf{k})$ into account. The effect of EC in σ_{xx} is more sensitive than in σ_{zz}, as shown

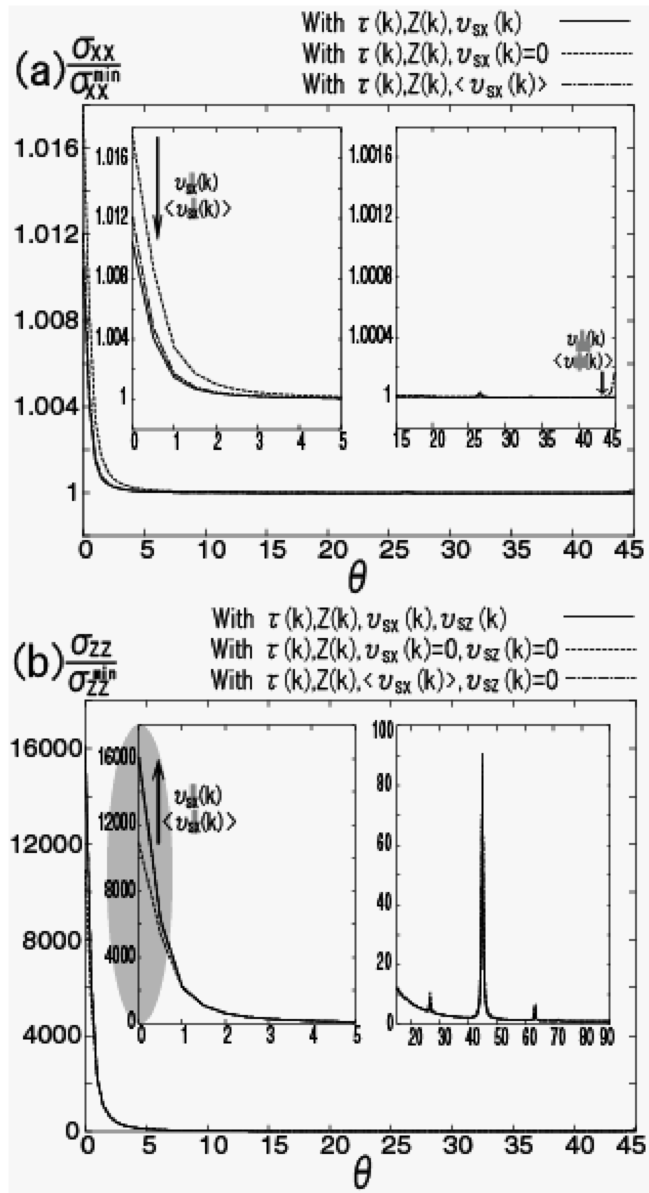

Fig. 3. (a) Angle dependence of σ_{xx}. (b) Angle dependence of σ_{zz}. The solid lines mean the magnetoconductivities with using the momentum dependent $\tau(\mathbf{k})$, $Z(\mathbf{k})$ and $\upsilon_{sx}(\mathbf{k})$ (and $\upsilon_{sz}(\mathbf{k})$ in (b)). The dash lines indicate the magnetoconductivies in the case that the momentum dependence of $\upsilon_{sx}(\mathbf{k})$ (and $\upsilon_{sz}(\mathbf{k})$ in (b)) is neglected by using $\upsilon_{sx}(\mathbf{k}) = 0$ (and $\upsilon_{sz}(\mathbf{k}) = 0$ in (b)). The dash line with dot means the magnetoconductivies in the case that the constant component of $\upsilon_{sx}(\mathbf{k})$ is treated by using $\langle\upsilon_{sx}(\mathbf{k})\rangle$ (and $\upsilon_{sz}(\mathbf{k}) = 0$ in (b)).

in Figs. 1(a) and 1(b). The effect is small at other angles $\theta = 26.4°$ and $45°$. In Fig. 3(b), the strong enhancement at $\theta = 0°$ is obtained in the calculation of $\sigma_{zz}(\mathbf{k})$ by neglecting only $\upsilon_{sz}(\mathbf{k})$ and the momentum dependence of $\upsilon_{sx}(\mathbf{k})$ (Using $\upsilon_{sz}(\mathbf{k}) = 0$ and the averaged value $\langle\upsilon_{sx}(\mathbf{k})\rangle$.), while the enhancement is not obtained in the calculation by neglecting only $\upsilon_{sz}(\mathbf{k})$ and $\upsilon_{sx}(\mathbf{k})$ ($\upsilon_{sz}(\mathbf{k}) = 0$ and $\upsilon_{sx}(\mathbf{k}) = 0$.). Therefore, the results indicate that σ_{zz} is also enhanced at $\theta = 0$ when we calculate it with using only the average $\langle\upsilon_{sx}\rangle$, whereas the effect of $\langle\upsilon_{sz}(\mathbf{k})\rangle$ on σ_{zz} is very small. The enhancement in the peak of σ_{zz} at $\theta = 0°$ is caused by the increase in veloc-

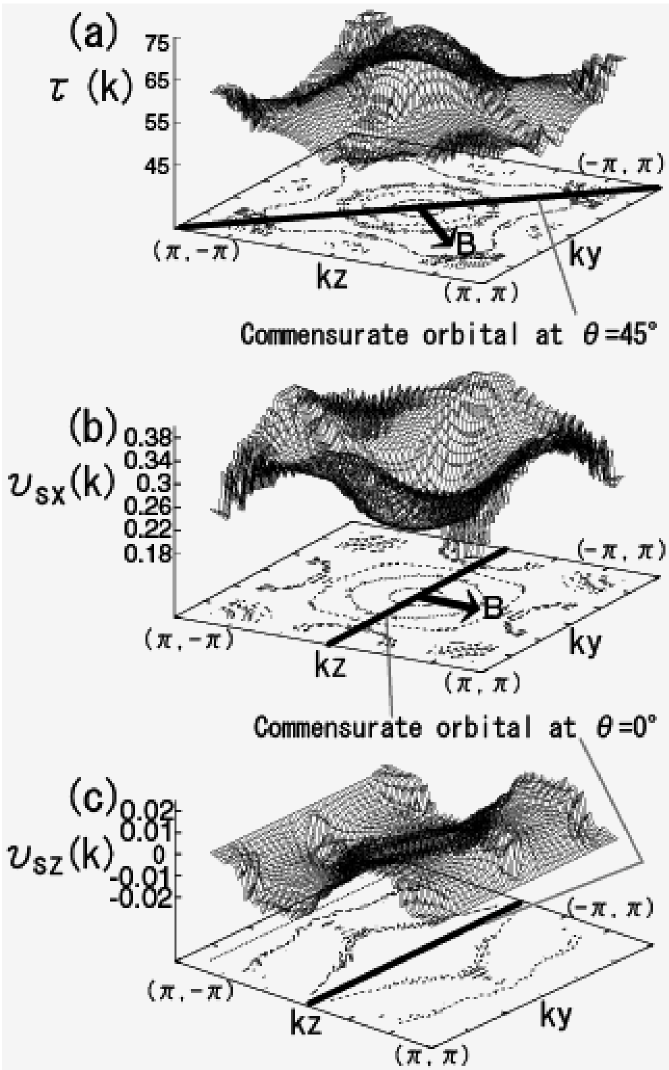

Fig. 4. (a) $\tau(\mathbf{k})$, (b) $v_{sx}(\mathbf{k})$ and (c) $v_{sz}(\mathbf{k})$ on FS and commensurate orbitals at a magic angles 45° and 0°.

ity due to $v_{sx}(\mathbf{k})$. EC increases the velocity $v_x(\mathbf{k})$. The averaged value $\langle v_{sx}(\mathbf{k})\rangle$ is 0.3, as shown in Fig. 4(b). The effect of $v_{sz}(\mathbf{k})$ on σ_{zz} is very small because $\langle v_{sz}(\mathbf{k})\rangle$, as shown in Fig. 4(c), equals 0.

Here, the effects of v_{sx} suppress the peak at 0° in σ_{xx} as shown in Fig. 3(a), whereas the momentum dependence of $\tau(\mathbf{k})$ enhances the peak as shown in Fig. 2(a). Therefore, the change of the peak at 0° by EC does not appear in the case (Fig. 1(a)) when the both effects exist.

The reason why $\tau(\mathbf{k})$ suppresses σ_{xx} at $\theta = 45°$ is explained as follows. On the peak of $\theta = 45°$ in σ_{xx}, the momentum dependence of $\tau(\mathbf{k})$ over the commensurate orbitals disturbs the momentum dependence of $v_x(\mathbf{k})$ which causes peaks in σ_{xx} at magic angles. The peak at $\theta = 45°$ is suppressed by the electron-electron scattering due to the momentum dependence of lifetime, which originates from EC near the SDW, over the commensurate orbital.

Next, the enhancement in σ_{zz} at $\theta = 0°$ by $\langle v_{sx}(\mathbf{k})\rangle$ is explained as follows. The increase of velocity due to $\langle v_{sx}(\mathbf{k})\rangle$[19] near the SDW connects to the pseudo gap, which indicates the decrease of the density of state ($\frac{1}{v_x(\mathbf{k})}$ in eq. (6)), due to spin fluctuation.[20] The decrease in the density of states suppresses the amplitude of the momentum dependence of $v_x(\mathbf{k})$, which changes the overlap of the momentum dependences of $\frac{v_z(\mathbf{k}(0))}{v_x(\mathbf{k}(0))}$ and $v_z(\mathbf{k}(t))$ in eq. (6). The decrease in the amplitudes of $v_x(\mathbf{k})$ gives the small effect on the large amplitude of function in the momentum dependence of $\frac{v_z(\mathbf{k}(0))}{v_x(\mathbf{k}(0))}$ corresponding to the large peak at 0°, whereas it gives the large effect on the small amplitude of function corresponding to the small peaks at 26.4° and 45°. Therefore, the suppression of the large peak at 0° becomes weaker than the suppression of the peaks at the other magic angles of 26.4° and 45°.

To study the effect of the renormalization factor $Z(\mathbf{k})$, we calculate σ_{xx} and σ_{zz} by neglecting only the momentum dependence of $Z(\mathbf{k})$ using $\langle Z(\mathbf{k})\rangle$. We find that the effect of $Z(\mathbf{k})$ is very small in both σ_{xx} and σ_{zz}. The effect of $Z(\mathbf{k})$ is almost canceled in eqs. (5) and (6).

In comparison with the experimental results, we first comment on our results in σ_{zz}. The angular dependence is strong in σ_{zz} in the noninteracting system, whereas the relative height of peaks between magic angles does not agree with the experimental results. The effect of EC changes the relative height of the peaks in σ_{zz}, however the change is not sufficient to explain the experimental results. Next, we comment on σ_{xx}. In the Chaikin's simple model[12] of "hot spot", the strong angular dependence is obtained in 1D axis magnetoresistance, as observed experimentally. Zhelenyak and Yakovenko[13] have found that the variation of the lifetime on the Q1D FS calculated on the basis of Umklapp scattering is not strong enough to give the peaks in the 1D axis magnetoresistance for the model with linearized dispersion in the k_x-direction. In the present study, we did not linearize the dispersion and we found that EC changes the relative height of the peaks in the angular dependence of σ_{xx}. The heights of peaks, however, are not as high as those observed experimentally. One of the possible origins of the strong angle dependence may be the vertex corrections. Kontani[21] has shown that vertex correction plays an important role in the magnetoresistance of two-dimensional systems in the weak magnetic field. By using the quantum Kubo formula, the vertex correction should be taken into account in general, however, no formulation in the strong magnetic field has been obtained, as far as the authors know.

The Zeeman effect is not considered in this study. It will also affect the result, because $\chi_{\uparrow\uparrow}$, $\chi_{\downarrow\downarrow}$ and $\chi_{\uparrow\downarrow}$ are not the same in the presence of the Zeeman effect.

In summary, the momentum dependence of the quasiparticle's lifetime originating from EC near the SDW, which causes electron-electron scattering, suppresses σ_{xx} at the magic angle of 45°. The change of the quasiparticle's velocity due to EC, which connects to the pseudo gap due to spin fluctuation near the SDW, gives the enhancement in σ_{zz} at the magic angle 0°. The different effects of EC between the magic angles originate from the connection of the momentum dependences of lifetime and velocity with the momentum dependence of commensurate orbitals on a Fermi surface in magnetic fields at magic angles. The effect of EC is sensitive to

σ_{xx}. The effect of EC on AMRO may be considered as the origin of the deviation of the peak heights obtained in the experiments from that calculated in the noninteracting system.

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